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Title: Uncertainty Quantification in High Explosives Equations of State

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Uncertainty Quantification in High Explosives Equations of State

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Mentors: Jeff Leiding, Stephen Andrews, Chris Ticknor

XCP Computational Physics Student Summer Workshop
Final Presentations
August 10-12, 2021

Noah Lordi

Education

- Graduated Santa Clara University in 2020 with a bachelors in Physics and Mathematics
- Currently 2nd year Ph.D student in Physics at CU Boulder

Research Interests

- Quantum information theory
- Quantum Computation
- Quantum materials research

Jonathan Lindbloom

Education

- Graduated SMU ‘21 with Mathematics B.S., Finance B.B.A.
- Incoming Applied Mathematics doctoral student at Dartmouth College

Research Interests

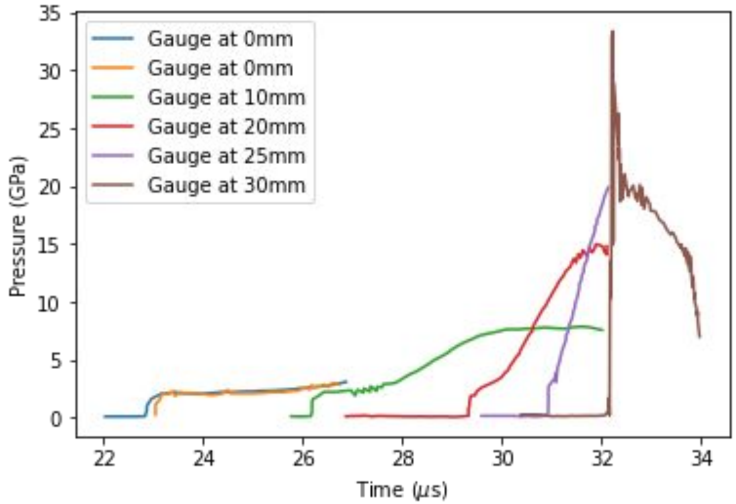
- Inverse problems + UQ
- Probabilistic machine learning
- Surrogate models

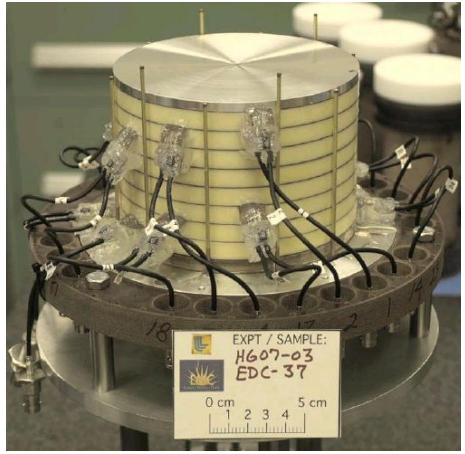
Simulation Validation and Uncertainty Quantification

- In order to fit models to data, we need a way to simulate the data given a model
- Our projects involved simulators for the Manganin gauge experiment and for cylinder tests, which we use to calibrate models to experiments
- We call the parameters we seek to optimize the degrees of freedom (DOF)
- We use a Bayesian approach with its associated UQ benefits

$$P(\theta|\mathcal{Y}) \propto P(\mathcal{Y}|\theta)P(\theta)$$

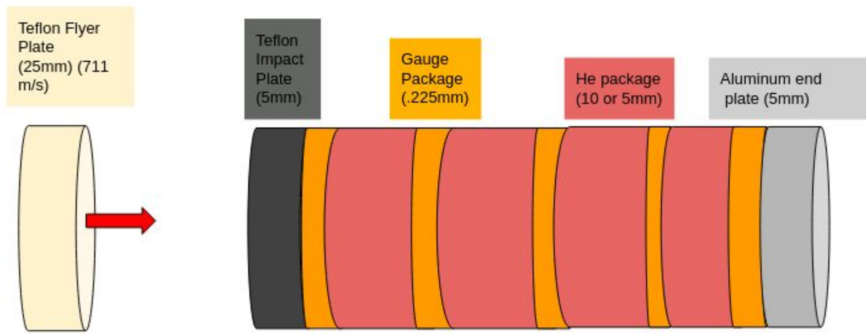
The Manganin Gauge Project





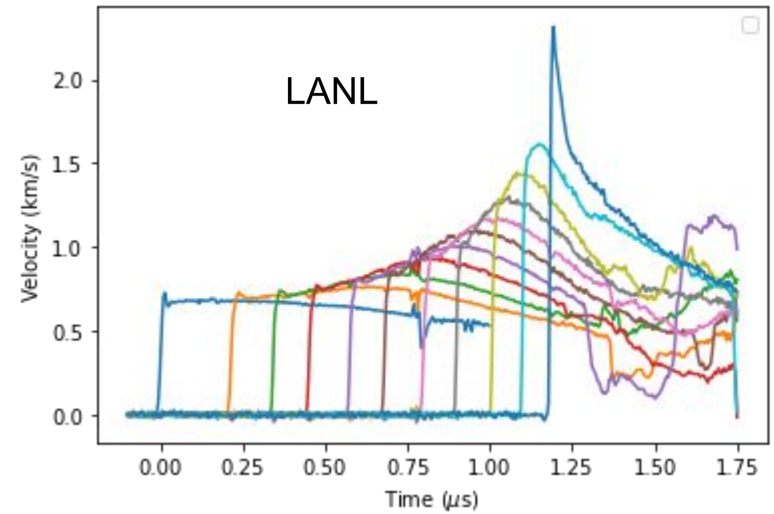
Experimental Setup

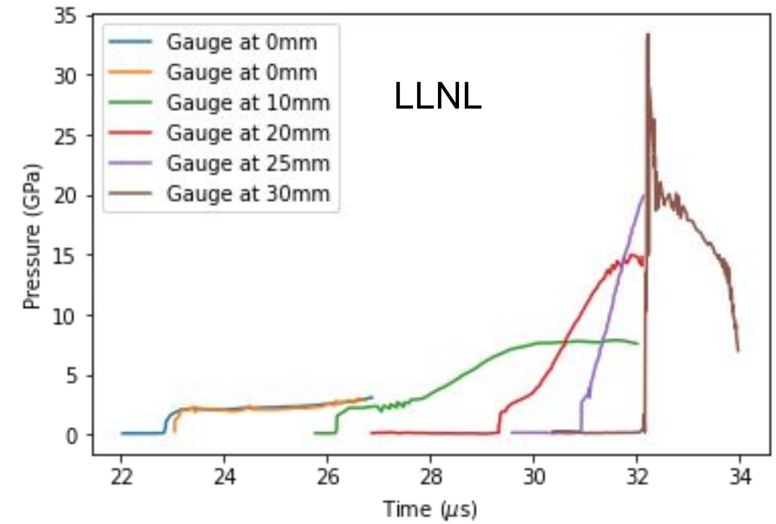
- Flyer plate impacts the setup to create an initial shock
- Shock Propagates at more than 3 km/s
- GPa pressure scales and microsecond time scales
- Supersonic shockwaves at detonation



Experimental Data

- This problem is very difficult to simulate
- Embedded gauge data from LANL is well studied
- LLNL has also run manganin gauge experiments
  - Historically hard to simulate
- Experimental setup is very similar
  - LLNL embeds gauges in teflon
    - Nontrivial wave-dynamics
- Want to incorporate LLNL data for EOS calibration and validation





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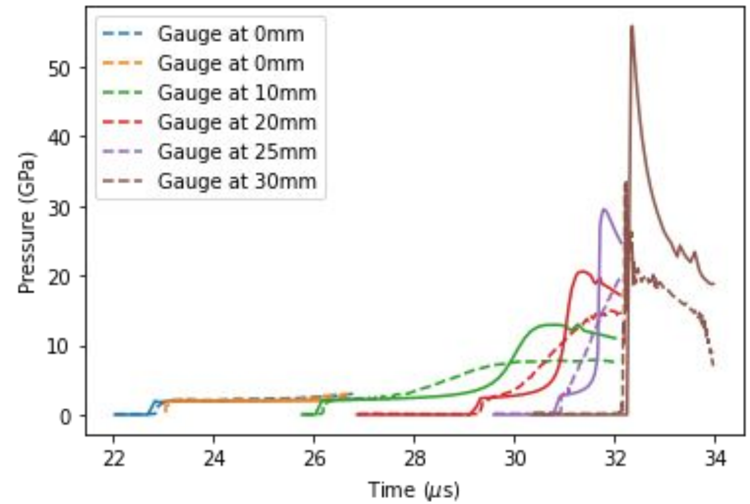
Direct Simulation Efforts

- Used a one dimensional unstable lagrangian (ODUL) solver within the ARISEE hydrocode
- Modeled the PBX9501 HE as a reactive flow
  - 26 parameters, 6 degrees of freedom (DOF)
- Initial values informed by previous research[2]
- Gets a lot correct
  - Predicts detonation



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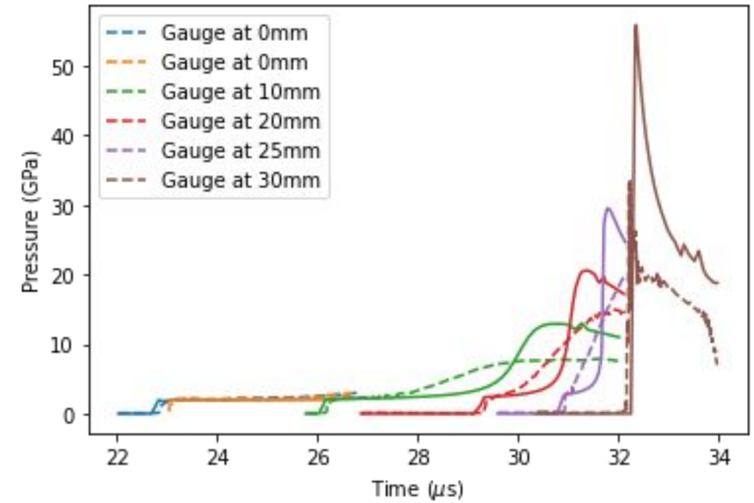
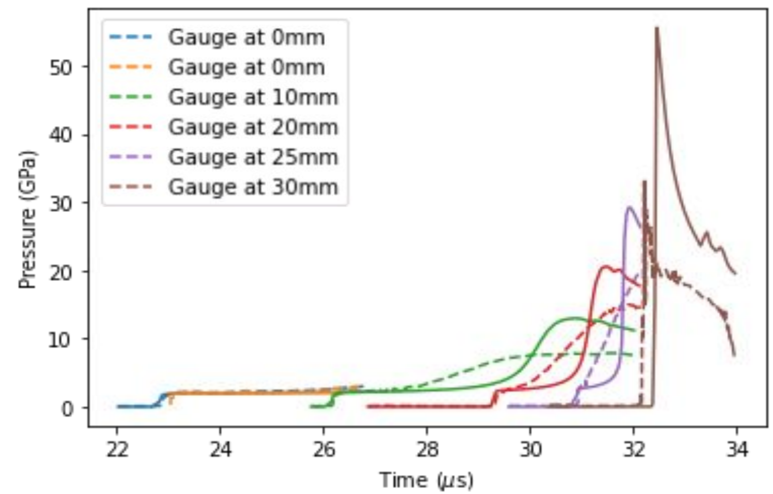
Simulation Optimization

- After one iteration of optimization we encounter a local minima
- Good qualitative agreement between simulation and experiment
- Want to compare to the LANL experiments





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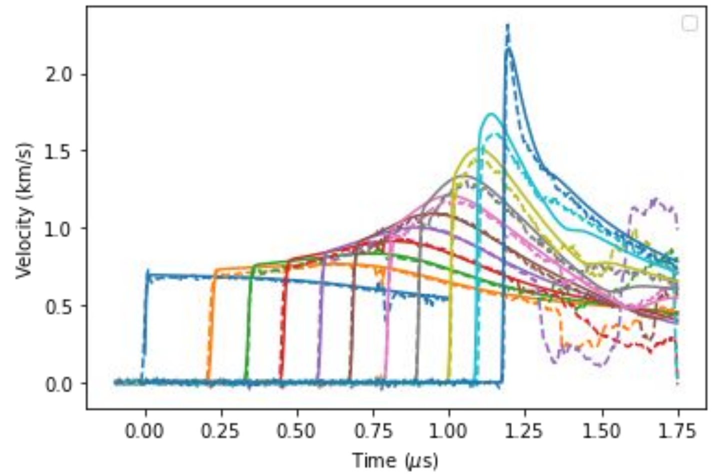
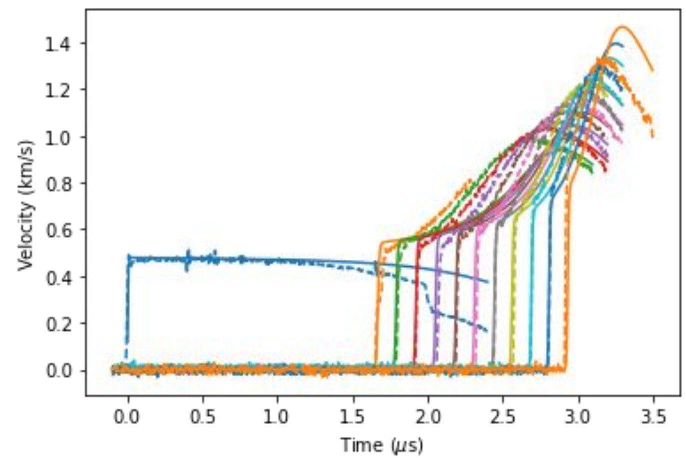
Comparing LANL and LLNL data

- Use the optimization scheme on the LANL experiments
  - Very good agreement
- Simultaneously optimize multiple experiments
- Thinner gauges and simpler wave mechanics
  - We trust this data
- These two LANL experiments are consistent
  - use same DOFs





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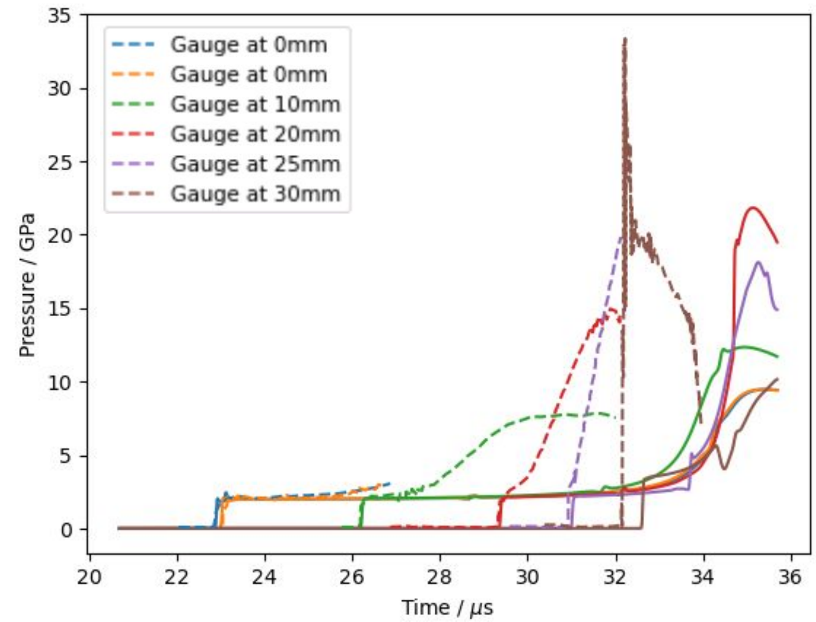
Validating the LLNL Data

- Using the DOFS from our previous optimizations
- LANL and LLNL data appear to be inconsistent
  - Different DOFS fit each experiment
  - Possible there is missing physics
- We are able to fit the LLNL data, but not as well as the LANL data



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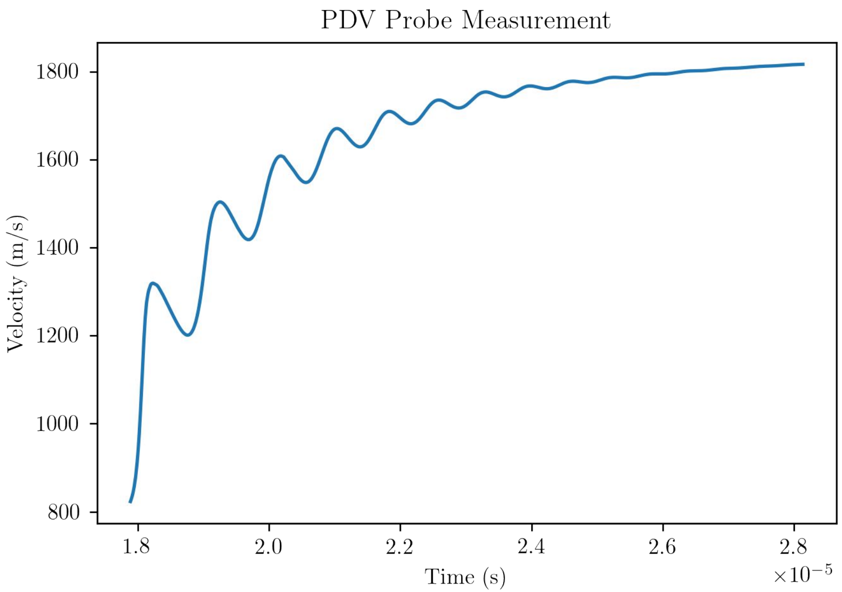
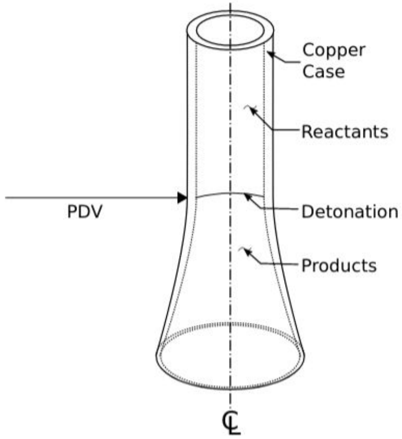
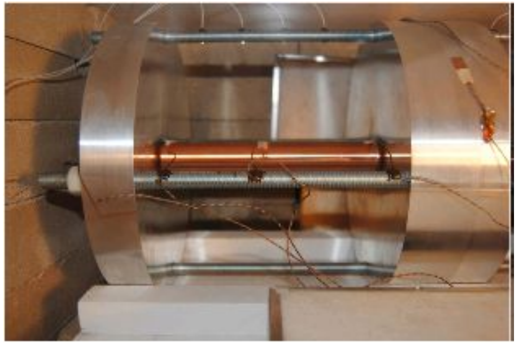
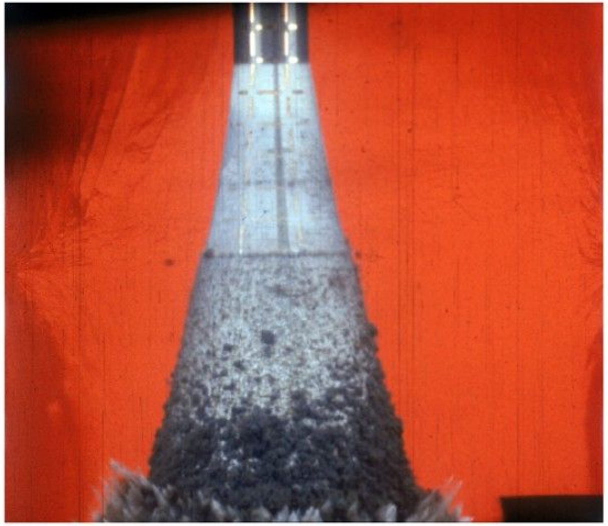
The Cylinder Test Project







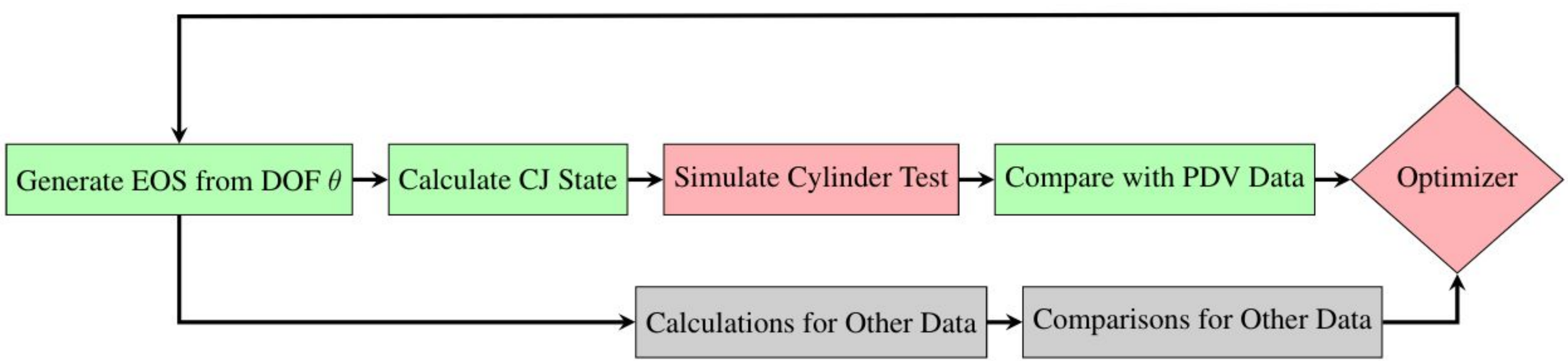


The CJ State

- The CJ state of a HE is the thermodynamic state at which the shock wave is sonic and the detonation is self-sustaining
- The CJ isentrope is the locus of thermodynamic states that the HE expands on during an explosion
- The CJ isentrope passes through the CJ state
- We cannot measure the entire CJ state directly, instead we view complicated functions of the CJ state (e.g. PDV probe data)

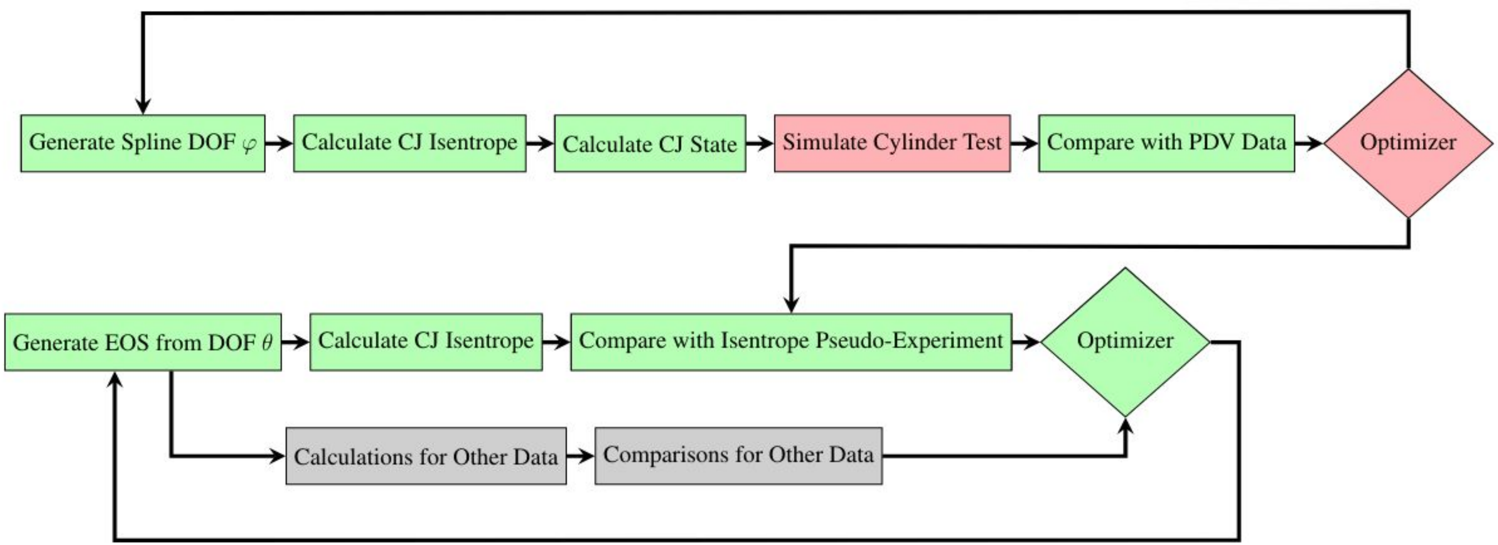
Simulating Cylinder Tests

- Running cylinder test simulations takes a long time (~45 minutes)
- Optimizers run many simulations to explore the parameter space (~2 days)
- Comparing errors in thermodynamic quantities is fast (< 1 second)
- Can we somehow avoid these simulations by extracting the information they contain upfront?



Proposed Workflow

- Cylinder tests inform the CJ isentrope
- Use a Gaussian process spline method to learn the CJ isentrope with uncertainties
- Calibrate EOS to this CJ isentrope pseudo-experiment instead of PDV data



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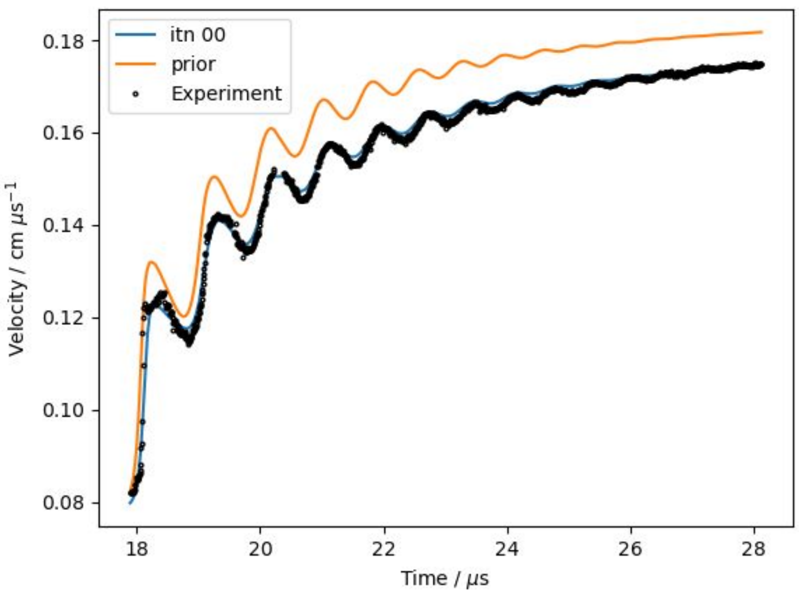
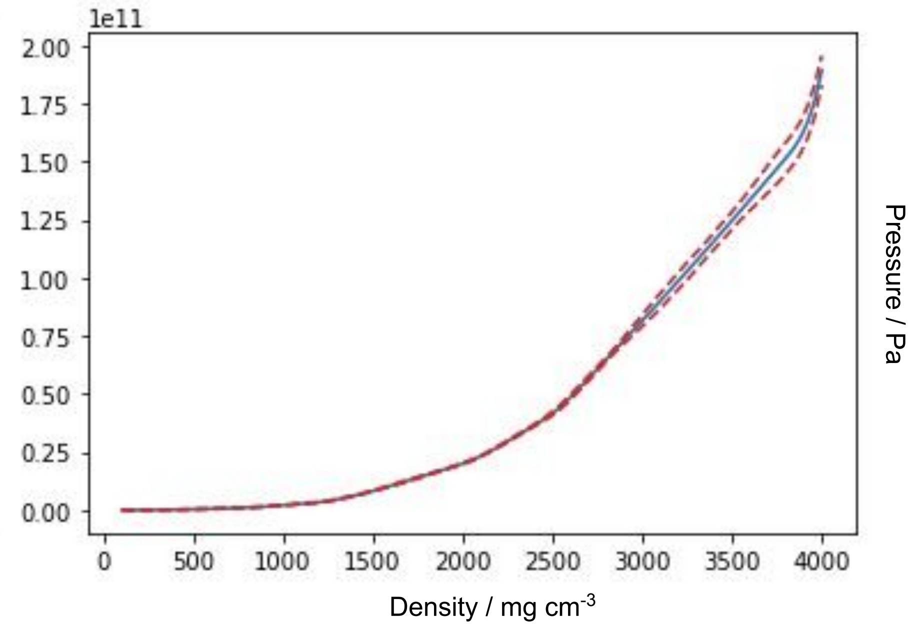
Benefits

- Fitting an EOS model becomes very fast (< 1 minute, instead of days) and permits uncertainty quantification for parameters and quantities of interest
- The learned CJ isentrope is agnostic towards any functional form
- We can fit many different parametric EOS models to the same CJ isentrope pseudo-experiment
- In principal we never need to run the cylinder test simulation again

Step 1: Invert the CJ Isentrope

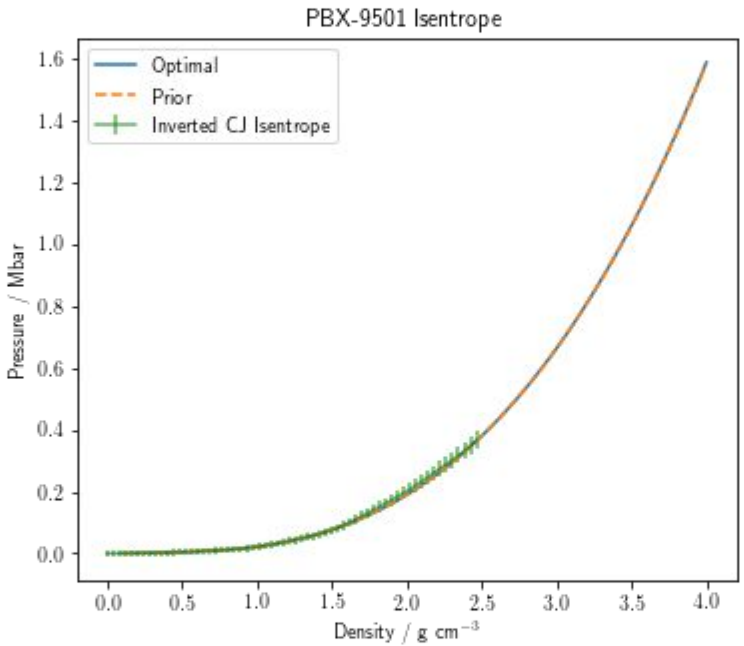
- Simulate many cylinder tests using varying proposal isentrope curves

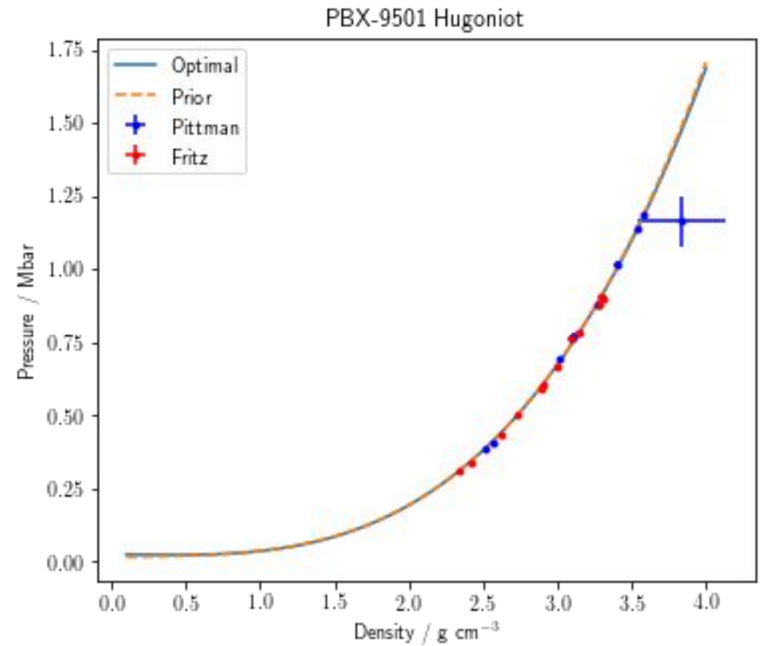




Step 2: Invert the EOS Model

- We use the Davis Products EOS
- Fit to CJ isentrope pseudo-experiment and overdriven Hugoniot data





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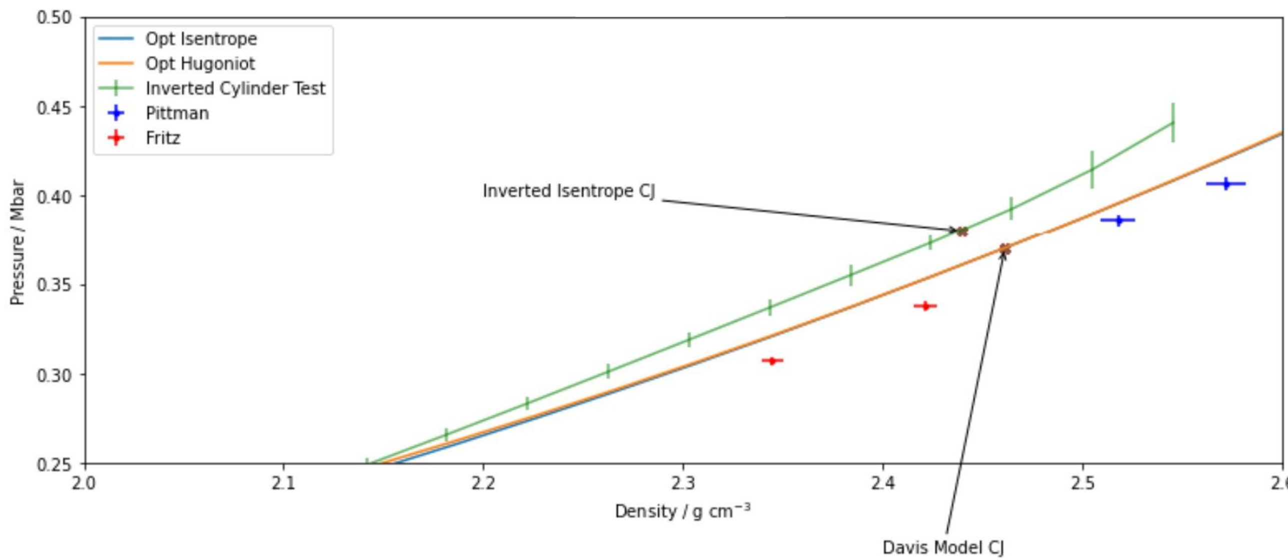
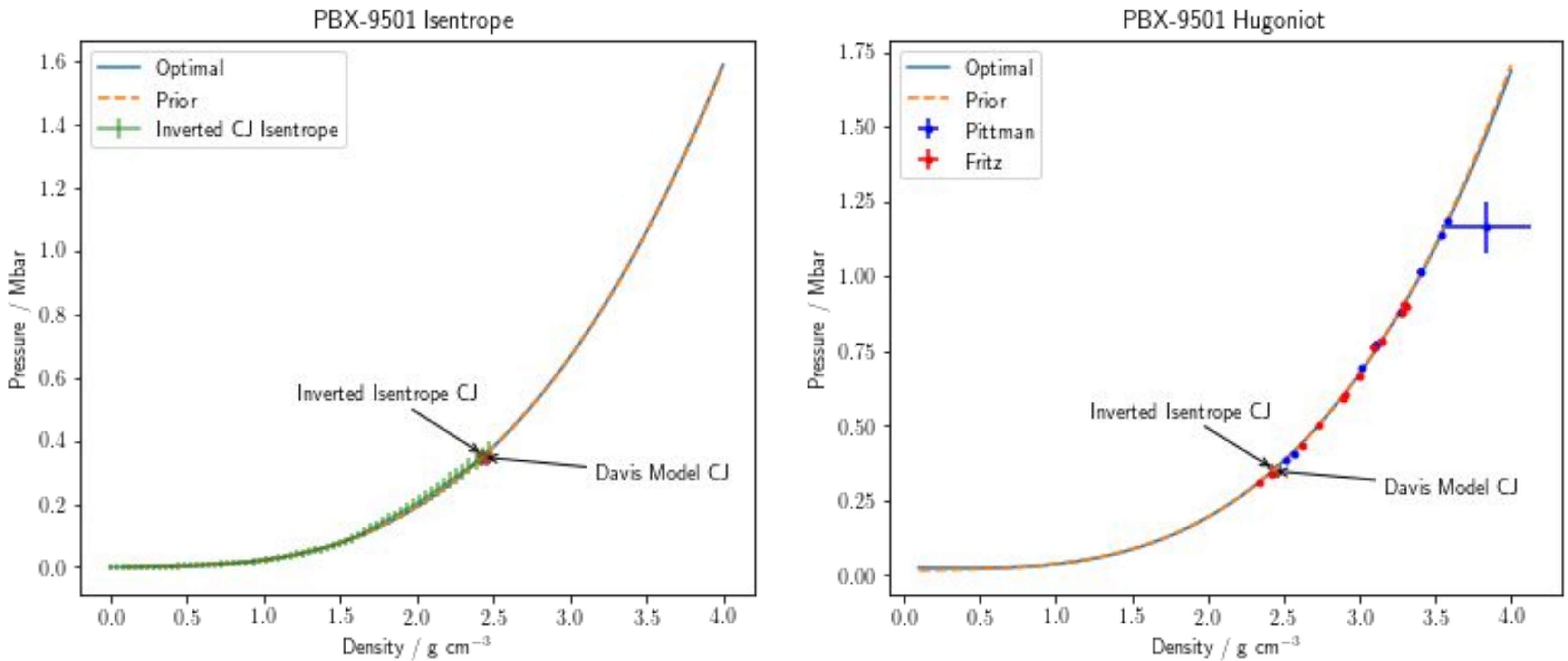
Conflicting CJ States

- Under this method, both the isentrope inversion and the EOS model infer a distribution over CJ states for the HE
- We remedy this by constraining the isentrope inversion by the observed detonation velocity, which was also measured during the cylinder test



Resulting Davis Products EOS Fit



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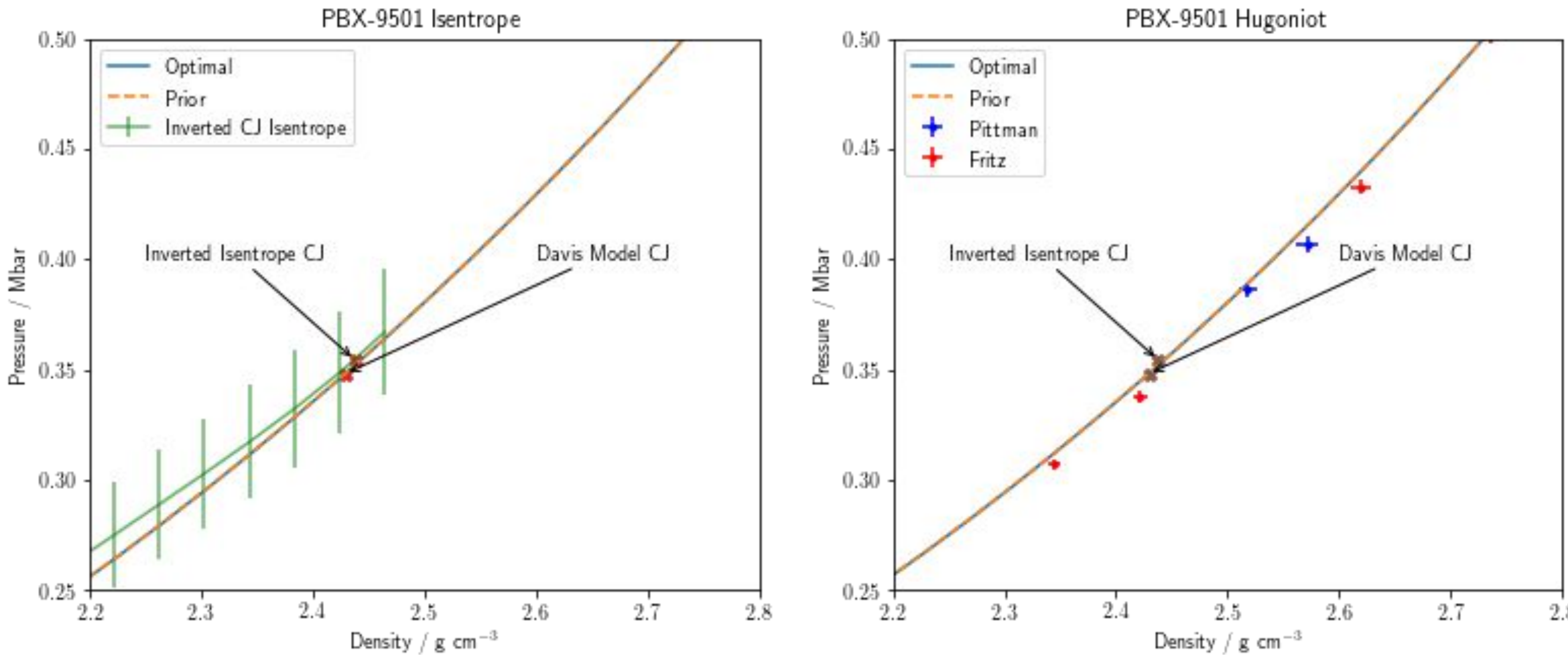
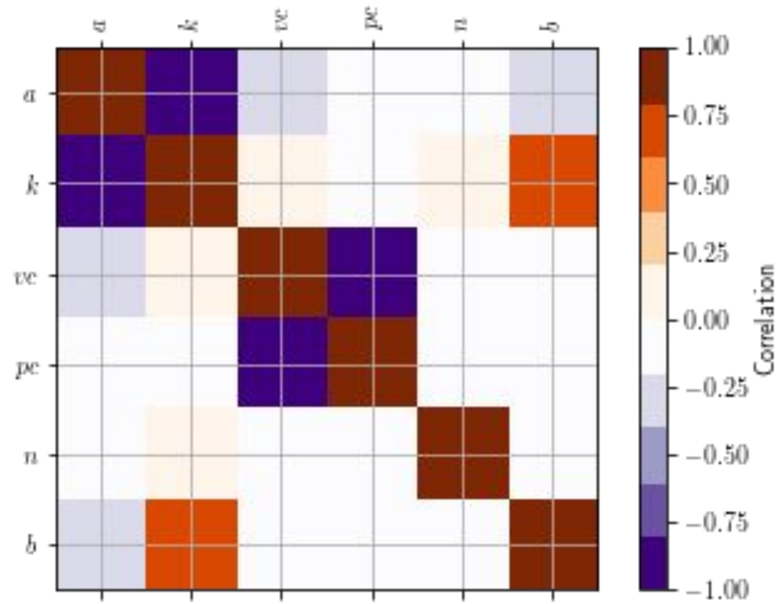
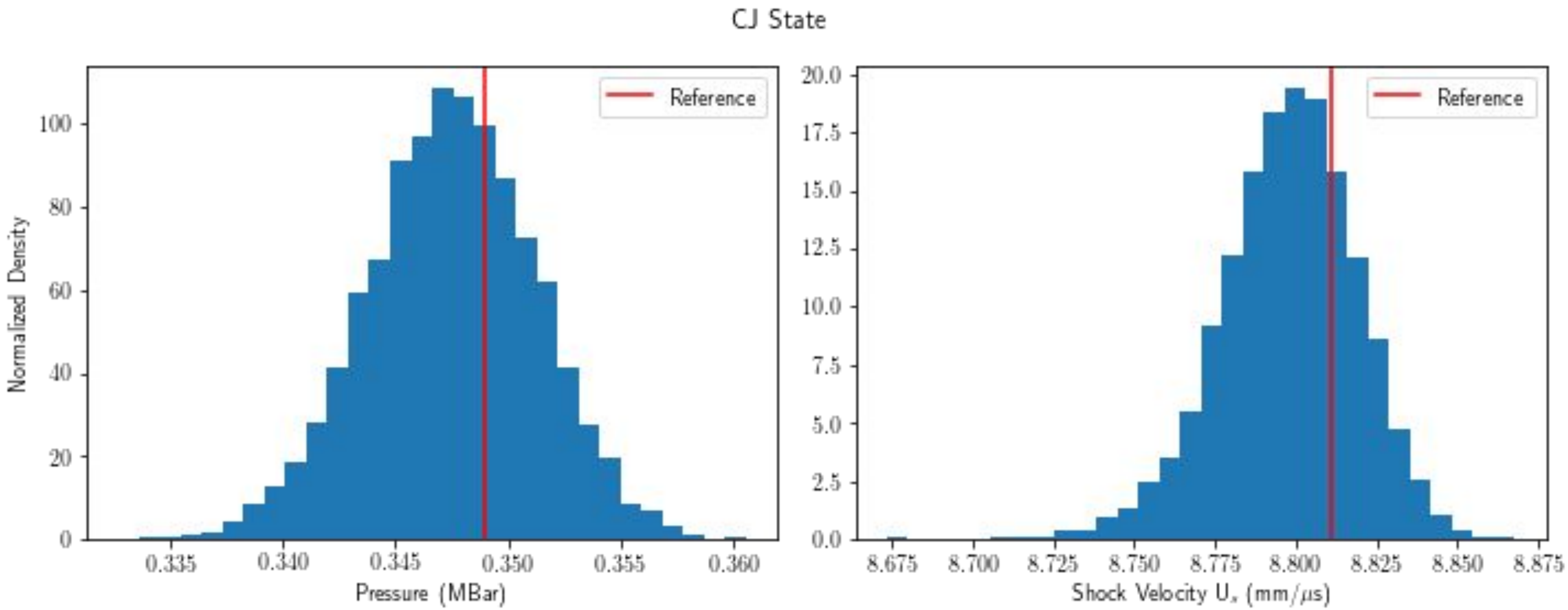


Uncertainty Quantification on Model DOF



Uncertainty Quantification on Model DOF



Conclusion

- The technique for inverting the CJ isentrope works well
- This introduces tension from two models inferring the CJ state independently
- Care must be taken to address conflicting CJ states
- The key benefit is that fitting EOS models downstream becomes fast
- Future work can explore the consistency of the cylinder test inversion across probes, shots, and experiments